Monte Carlo Simulations of Phase and Conformational Transitions in Complex Fluids (Invited)

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This presentation focuses on computational methodologies for simulations of phase equilibria and conformational transitions in fluids, as well as their applications. After a brief introduction to Gibbs ensemble and histogram-reweighting methods, we review recently developed intermolecular potential models for polar and non-polar components and discuss their predictive ability for mixtures. Recent work in our group demonstrating the equivalence of lattice and continuous-space models for non-polar and coulombic interactions will be summarized. The controlling parameter is the ratio of particle diameter to lattice spacing. For relatively low values of this parameter, coexistence curves, critical parameters and liquid structure of lattice and continuous models are indistinguishable, but the lattice models are significantly more efficient computationally. Finally, applications of histogram-reweighting methods to aggregation and micellization in model surfactant solutions will be presented. Connections between the models and real surfactant solutions can be made through mapping of their phase behavior. Near-quantitative agreement is found for the critical micelle concentration (cmc), but the temperature dependence of the cmc is incorrect, suggesting the need to incorporate more realistic solvent models.